

# Index

## A

Axial vector, crystallographic point groups, 61–62

## B

Basis functions, 31

Birefringence, 114–118

Bloch wave function, 216–218

Bravais lattices, 6

Brillouin zones, 21–23

## C

Cartesian coordinates transformation, 28–29

Character table

32 crystallographic point groups, 32–38

Pauli spin operators, 39–40

Coordinates transformation matrix, 29

Crystal field symmetry

medium crystal field case, 86

octahedral coordination, ligands, 86–87

perturbation theory, 86

Stark splitting, 85

strong crystal field case, 86

weak crystal field case, 85

Crystals optical properties and symmetry

birefringence

crystal dielectric property, 114–115

double refraction, 115

indicatrix, 116–117

linear optics fundamental equation, 115–116

optically anisotropic material properties, 118

uniaxial crystal, wave surface, 118

electrooptical effect

crystallographic point groups,

electrooptic tensor, 126

crystallographic point groups, Kerr tensor, 130–131

crystals electrooptic coefficients, 127

$C_{3v}$  symmetry crystal electric field, 129

$D_{2d}$  symmetry electrooptic tensor, 128

first-order electrooptic effect/Pockels effect, 123–124

Kerr coefficients, 129

Kerr effect, 124–125

optical activity

definition, 118

gyration tensor, 120

gyration tensor crystallographic point groups, 122–123

Neumann's principle, 122

rotatory dispersion effect, 121

rotatory power, 119

spatial dispersion, 119

symmetry properties, gyration tensor components, 122

photoelastic effect

elasto-optical coefficients, 134

photoelastic tensor-tensor form

difference, 133

piezooptical coefficients, 131

refractive index coefficients, 132

polarization, tensor treatment

electromagnetic light wave, electric field, 106

Jones matrices, 112

Jones vector, 110–111

left-circularly polarized light, 107

light wave electric field, 106–107

Mueller matrices, 113, 114

polarization transformation matrices, 113

polarization vectors, 109

- polarization (*cont.*)  
 polarized light, 108  
 right-circularly polarized light, 107  
 state of, 105–106  
 Stokes parameters, 107–108
- Crystal structure  
 axes type, 9  
 Bravais lattices, 6  
 crystal lattice types, 5  
 cubic system, 10  
 3D crystal lattice, 6–8  
 hexagonal system, 10  
 monoclinic system, 9  
 noncubic crystallographic point groups, 11–13  
 O and  $O_h$  crystallographic point groups, 14  
 orthorhombic system, 9  
 primitive unit cell, 4  
 space groups, 12  
 square lattice, 4–5  
 stereograms, 10  
 symmorphic space group, 5  
 tetragonal system, 9  
 tetrahedral symmetry, 14–15  
 triclinic and trigonal systems, 9
- Crystal tensor properties  
 first-rank matter tensors  
 axial vector, crystallographic point groups, 61–62  
 crystallographic point groups, 59  
 crystal spatial rotation effect, 57–58  
 ferroelectric effect, 60  
 ferromagnetic effect, 61  
 nonferroelectric-ferroelectric crystals correlation, 60  
 pyroelectric effect, 57  
 pyroelectric-ferroelectric phenomena difference, 60  
 pyroelectric tensor, 58–59  
 scalar cause, vector effect, 57  
 fourth-rank matter tensors  
 crystallographic point groups, 76–77  
 elastic compliance, 74  
 elastic compliance components, 75  
 Hooks's law, 74  
 Neumann's principle, 55  
 second-rank matter tensors  
 cause and effects, 62  
 conductivity tensor, 63  
 crystallographic point groups, 66  
 cubic point group symmetry operation, 65  
 electrical conductivity, 63  
 four-fold rotation symmetry, 64  
 nonzero elements, conductivity tensor, 65  
 quadratic equation, coordinate system, 66  
 temperature-induced deformation, 67–68  
 Taylor series, 56  
 third-rank matter tensors  
 crystallographic point groups, 72–73  
 mirror reflection matrix, 71  
 piezoelectric effect, 68  
 piezoelectric tensor, 69–70  
 stress sensor components, 68–69  
 symmetry transformation properties, 70
- D**
- d-electrons  
 applications, 95–96  
 $Cr^{3+}$  ion electric dipole transitions, 99  
 $Cr^{3+}$  ion energy levels, 99  
 crystal field energy determination, 99–100  
 $O_h$  crystal field optical transitions, 96  
 $O_h$  symmetry group, 97  
 $O$  symmetry free ions, 98
- E**
- Elastic compliance, 74  
 Electron energy bands  
 Bloch wave function, 216–218  
 cyclic groups, concepts, 215  
 energy vs. wave vector, 219  
 Electrooptical effect  
 crystallographic point groups  
 electrooptic tensor, 126  
 Kerr tensor, 130–131  
 crystals electrooptic coefficients, 127  
 $C_{3v}$  symmetry crystal electric field, 129  
 $D_{2d}$  symmetry electrooptic tensor, 128  
 first-order electrooptic effect/Pockels effect, 123–124  
 Kerr coefficients, 129  
 Kerr effect, 124–125
- F**
- f-electrons  
 $C_{kq}$  spherical harmonics, 101–102  
 Judd–Ofelt theory, 103–104  
 $Nd^{3+}$  energy levels, 103  
 $Nd^{3+}$  selection rule, 103  
 point group  $D_{2d}$  character table, 102  
 rare earth ions, 100  
 spin–orbit coupling splits, 101

- First-order electrooptic effect, 123–124
- First-rank matter tensors
- axial vector, crystallographic point groups, 61–62
  - crystallographic point groups, 59
  - crystal spatial rotation effect, 57–58
  - ferroelectric effect, 60
  - ferromagnetic effect, 61
  - nonferroelectric-ferroelectric crystals
    - correlation, 60
  - pyroelectric effect, 57
  - pyroelectric-ferroelectric phenomena
    - differences, 60
  - pyroelectric tensor, 58–59
  - scalar cause, vector effect, 57
- Fourth-rank matter tensors
- crystallographic point groups, 76–77
  - elastic compliance, 74
  - elastic compliance components, 75
  - Hook's law, 74
- G**
- Group theory
- basis functions, 31
  - Cartesian coordinates transformation, 28–29
  - character table
    - 32 crystallographic point groups, 32–38
    - Pauli spin operators, 39–40
  - concept, 26
  - coordinates transformation matrix, 29
  - definition, 25
  - order of group, 25–26
  - physical properties, system, 27–28
  - point group symmetry, 27
  - properties, 26
  - quantum mechanics
    - eigenfunctions  $E_i$ , 50
    - eigenvalue  $E_n$ , 49
    - rectangular symmetry, 52–53
    - Schrödinger equation, 48
    - spatial and spin functions, 51
    - spin-orbit interaction, 51
  - trace, transformation matrix, 30
- Gyration tensor, 120
- H**
- Hook's law, 74
- J**
- Jahn–Teller effect, 194–197
- Jones matrices, 112
- Jones vector, 110–111
- Judd–Ofelt theory, 103–104
- K**
- Kerr coefficients, 129
- Kerr effect, 124–125
- Kleinman symmetry, 147
- L**
- Lattice vibrations
- acoustic mode, 173
  - Brillouin zone symmetry operation, 177
  - $O_h$  and  $C_{4v}$  point groups, 179
  - optic mode, 173
  - phonon dispersion, 180
  - $\text{SrTiO}_3$  Brillouin zone, 174–176, 178–179
  - strontium titanate ( $\text{SrTiO}_3$ ) crystal
    - structure, 173–174
- Legendre polynomials, 222–223
- Light wave electric field, 106–107
- M**
- Maxwell's wave equation, 141
- Mueller matrices, 113, 114
- N**
- Neumann's principle, 55
- Nonlinear optics
- birefringence, 144
  - Clausius–Mossotti relationship, 137
  - controlling parameters, phase mismatch, 143
  - coordinate system, 144–145
  - coupled wave equation, 141–142
  - effective nonlinear optical coefficient
    - coordinate system, ordinary and extraordinary polarization vectors, 147–149
  - crystallographic point groups, 148, 149
  - fourfold rotation, z-axis, 146
  - Kleinman symmetry, 147
  - nonlinear optical tensor, 146
  - tensor component expression, 145–146
- frequency doubling, 138
- index matching, 150–153
- materials, 137
- Maxwell's wave equation, 141
- momentum conservation, 140
- Raman scattering, 138
- second-harmonic generation, 139
- beam, 143
  - conversion efficiency, 142
  - photon transitions, 139
  - polarization, 139–140

- second-harmonic generation (*cont.*)  
 power, phase mismatch, 142  
 SHG efficiency maximizing  
 noncritical phase matching, 155  
 positive crystal,, 156–157  
 type I phase matching, 153–154  
 uniaxial negative crystals, 155  
 standard approach, 138–139  
 two-photon absorption  
 laser source producing photons, 157  
 $O_h$  point group character table, 38, 161  
 optical transitions, 159–160  
 symmetry properties, excited states, 159  
 tool, 158–159  
 uniaxial crystal propagation direction, 143, 144
- O**  
 Order of group, 25–26
- P**  
 Pauli spin operators, 39–40  
 Photoelastic effect  
 elasto-optical coefficients, 134  
 photoelastic tensor-tensor form difference, 133  
 piezo-optical coefficients, 131  
 refractive index coefficients, 132  
 Pockels effect, 123–124  
 Point group symmetry, 27  
 Polarization, tensor treatment  
 electromagnetic light wave, electric field, 106  
 Jones matrices, 112  
 Jones vector, 110–111  
 left-circularly polarized light, 107  
 light wave electric field, 106–107  
 Mueller matrices, 113, 114  
 polarization transformation matrices, 113  
 polarization vectors, 109  
 polarized light, 108  
 right-circularly polarized light, 107  
 state of, 105–106  
 Stokes parameters, 107–108  
 Polarizability tensor, 186  
 Primitive unit cell, 4  
 Pyroelectric effect, 57  
 Pyroelectric tensor, 58–59
- Q**  
 Quantum mechanics, in group theory  
 eigenfunctions  $E_i$ , 50  
 eigenvalue  $E_n$ , 49
- rectangular symmetry, concept, 52  
 rectangular symmetry, irreducible representations, 52–53  
 Schrödinger equation, 48  
 spatial and spin functions, 51  
 spin-orbit interaction, 51
- R**  
 Raman tensor, 188  
 Raman scattering  
 32 crystallographic point groups, Raman tensor, 188–193  
 material effects and applications, 194  
 Raman spectroscopy, 186  
 schematic picture, infrared absorption, 187–188  
 Stokes scattering, 185  
 Rayleigh scattering, 186  
 Reciprocal space  
 Brillouin zones, 21–23  
 description, 15  
 hexagonal crystal structure, 23  
 lattice periodicity function, 22  
 primitive translation vectors, 21  
 real and reciprocal space, equivalent lattices, 22, 23  
 space group list, 16–20  
 Rotatory dispersion effect, 121
- S**  
 Schoenflies notation, 9, 14, 15  
 Second-rank matter tensors  
 cause and effects, 62  
 conductivity tensor, 63  
 crystallographic point groups, 66  
 cubic point group symmetry operation, 65  
 electrical conductivity, 63  
 four-fold rotation symmetry, 64  
 nonzero elements, conductivity tensor, 65  
 quadratic equation, coordinate system, 66  
 temperature-induced deformation, 67–68  
 Solids point defects, symmetry properties  
 crystal field symmetry  
 medium crystal field case, 86  
 octahedral coordination, ligands, 86–87  
 perturbation theory, 86  
 Stark splitting, 85  
 strong crystal field case, 86  
 weak crystal field case, 85  
 crystal, ions energy levels  
 Cartesian coordinates, 92  
 crystal field matrix elements, 94  
 crystal field splitting, 95

- d-electron, energy level splitting, 90
- double-valued representation, 89
- forced electric dipole transitions, 91
- group theory, 91
- nonrotational symmetry elements,
  - transformation matrix, 89
- nonzero expansion coefficients, 93
- orbital angular momentum quantum, 87
- $O$  symmetry crystal field, 90
- principal symmetry axis, 88
- rotation operator, 88
- secular determinant elements, 95
- specific linear combination
  - determination, 92
- d-electrons
  - applications, 95–96
  - $\text{Cr}^{3+}$  ion electric dipole transitions, 99
  - $\text{Cr}^{3+}$  ion energy levels, 99
  - crystal field energy determination,
    - 99–100
  - $O_h$  crystal field optical transitions, 96
  - $O_h$  symmetry group, 97
  - $O$  symmetry free ions, 98
- f-electrons
  - $C_{kq}$  spherical harmonics, 101–102
  - Judd–Ofelt theory, 103–104
  - $\text{Nd}^{3+}$  energy levels, 103
  - $\text{Nd}^{3+}$  selection rule, 103
  - point group  $D_{2d}$  character table, 102
  - rare earth ions, 100
  - spin–orbit coupling splits, 101
- free ions energy level
  - angular momentum operators, 81
  - Coulomb interactions, 79
  - electron–electron interaction, 83
  - Hamiltonian representation, 80
  - spectroscopic notation, 82
  - spherical harmonic functions, 83–85
  - spin–orbit coupling constant, 82
  - spin–orbit interaction, 82–83
- Solid symmetry
  - concept, 2
  - crystal structure
    - axes type, 9
    - Bravais lattices, 6
    - crystal lattice types, 5
    - cubic system, 10
    - 3D crystal lattice, 6–8
    - hexagonal system, 10
    - monoclinic system, 9
    - noncubic crystallographic point groups,
      - 11–13
    - $O$  and  $O_h$  crystallographic point groups,
      - 14
    - orthorhombic system, 9
    - primitive unit cell, 4
    - space groups, 12
    - square lattice, 4–5
    - stereograms, 10
    - symmorphic space group, 5
    - tetragonal system, 9
    - tetrahedral symmetry, 14–15
    - triclinic system, 9
    - trigonal system, 9
  - definition, 1
  - elements, 2–3
  - group theory, 3
  - reciprocal space
    - Brillouin zones, 21–23
    - description, 15
    - hexagonal crystal structure, 23
    - lattice periodicity function, 22
    - primitive translation vectors, 21
    - real and reciprocal space, equivalent
      - lattices, 22, 23
    - space group list, 16–20
    - square array, elements, 3
- Space group list, 16–20
- Stokes parameters, 107–108
- Strontium titanate ( $\text{SrTiO}_3$ )
  - Brillouin zone, 174–176, 178–179
  - crystal structure, 173–174
- Symmetry and electron energy levels
  - electron energy bands
    - Bloch wave function, 216–218
    - cyclic groups, concepts, 215
    - energy  $vz$  wave vector, 219
  - molecular bonds
    - Cartesian and spherical coordinates
      - relationship, 201–202
    - $D_{3h}$  symmetry,  $\text{AB}_3$  molecule, 206–208
    - $D_{3h}$  symmetry group character table,
      - 205–206
    - $d_{yz}$  orbital, p bonding, 211
    - hybrid orbitals, 203
    - molecular orbitals, 208–209
    - $O_h$  symmetry orbitals molecules,
      - 209–211
    - s, p, and d electron orbitals, angular
      - factors, 202
    - spatial distribution, s, p, and d electron
      - orbitals, 202–203
    - $T_d$  point group character table,
      - 204–205

- molecular bonds (*cont.*)  
 tetrahedral molecule  $T_d$  symmetry, 203–204  
 space groups character tables, 212–214  
 symmetry property, electron energy bands  
 Brillouin zone, delta point, 220  
 Brillouin zone octahedral crystal symmetry, 221  
 group, wave vector, 220  
 Legendre polynomials, 222–223  
 many-body problem, 223
- Symmetry and lattice vibrations  
 Jahn–Teller effect, 194–197  
 lattice vibration mode  
 acoustic mode, 173  
 Brillouin zone symmetry operation, 177  
 $O_h$  and  $C_{4v}$  point groups, 179  
 optic mode, 173  
 phonon dispersion, 180  
 $SrTiO_3$  Brillouin zone, 174–176, 178–179  
 strontium titanate ( $SrTiO_3$ ) crystal structure, 173–174
- local mode vibrations  
 breathing mode, 171  
 definition, 166  
 normal vibration mode, 168–170  
 octahedral configuration, 166  
 $O_h$  character table for point group, 166, 167  
 $O_h$  symmetry  $r_1$  coordinates transformation, 170, 171  
 $\theta_{15}$  coordinate- $O_h$  symmetry transformation, 171, 172  
 symmetry coordinates, 168  
 phonons, 165  
 Raman scattering  
 32 crystallographic point groups, Raman tensor, 188–193  
 material effects and applications, 194  
 polarizability tensor, 186  
 Raman spectroscopy, 186  
 Raman tensor, 188  
 Rayleigh scattering, 186  
 schematic picture, infrared absorption, Raman scattering, 187–188  
 Stokes scattering, 185
- T**  
 Taylor series, 56  
 Temperature-induced deformation, 67–68  
 Third-rank matter tensors  
 crystallographic point groups, 72–73  
 mirror reflection matrix, 71  
 piezoelectric effect, 68  
 piezoelectric tensor, 69–70  
 stress sensor components, 68–69  
 symmetry transformation properties, 70
- Two-photon absorption  
 laser source producing photons, 157  
 $O_h$  point group character table, 38, 161  
 optical transitions, 159–160  
 symmetry properties, excited states, 159  
 tool, 158–159
- U**  
 Uniaxial negative crystals, 155
- V**  
 Vibrational energy level transitions  
 infrared transitions, 183–185  
 radiationless processes, 180  
 radiationless transitions, 181–183